

IN THE CLAIMS:

The text of all pending claims (including withdrawn claims) is set forth below. Cancelled and not entered claims are indicated with claim number and status only. The claims as listed below show added text with underlining and deleted text with ~~strikethrough~~. When strikethrough cannot easily be perceived, or when five or fewer characters are deleted, [[double brackets]] are used to show the deletion. The status of each claim is indicated with one of (original), (currently amended), (cancelled), (withdrawn), (new), (previously presented), or (not entered).

Please AMEND claims 16, 23 and 24 in accordance with the following:

1-15. (Cancelled)

16. (Currently Amended) A method of determining spatially similar portions of substances-a substance comprising amino acids by analyzing three-dimensional structures of a-the substance, by dividing a molecule of the substance into a plurality of target subsets based on secondary structures and comparing each of the plurality of target subsets of the molecule of the substance to a plurality of probe subsets of by-comparing a first probe structure, each of the plurality of probe subsets being expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets-of secondary structures of probe structures, the-wherein a first subset of the plurality of probe subsets comprising-comprises a first point set of an amino acid sequence database or a motif database and each of the plurality of target subsets is a target structure expressed by three-dimensional coordinates of elements belonging to a second subset of aof the plurality of target subsets of secondary structures of the-a target structure, wherein a first subset of the second-plurality of target subsets comprising-comprises a second point set of an input amino acid sequence of the target structure, wherein each point of the first point set and the second point set is expressed by three-dimensional coordinates and the coordinates are analyzed to determine correspondence, comprising:

dividing the second-target structure into a plurality of second-target subsets based on secondary structures of the three-dimensional coordinates of the target structure;

determining whether a correspondence is present between the first point set of the probe-structure-and the second point set of the plurality of second-subsets-of the target structure-by, for each subset of the plurality of target subsets of secondary structures of the target structure:

generating a first tree structure for the first point set of the probe structure-and a second tree structure for the second point set of the target structure wherein the tree structures are generated by successively giving correspondence to an element constituting the sets;

pruning the second tree structure for the second point set of the plurality of

~~second subsets of the target structure~~ in accordance with a predetermined pruning procedure; and

determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a the same attribute, generating a correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

calculating a root mean square distance (RMSD) value between elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure to automatically determine a value for a distance between the elements of the first point set and the elements of the second point set, wherein substances expressed by a point set $A = \{a_1, a_2, \dots, a_i, \dots, a_m\}$ of a target subset, and a point set $B = \{b_1, b_2, \dots, b_j, \dots, b_n\}$ of a probe subset, wherein a_i ($i=1, 2, \dots, m$) and b_j ($i=1, 2, \dots, n$) are vectors expressing positions of respective elements in three-dimensional space, elements constituting substances A and B are related to each other, and the substance B is rotated and moved so that the r.m.s.d. value between corresponding elements is minimized in accordance with a following equation (1) wherein U denotes a rotation matrix and W_k denote respective weights:

$$r.m.s.d. = \frac{\left(\sum_{k=1}^n (w_k (Ub_k - a_k)^2) \right)^{\frac{1}{2}}}{n} \quad \dots \dots (1);$$

determining whether the RMSD value is less than or equal to a predetermined threshold value set by a user, and where the RMSD value is less than or equal to a the predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure;

determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence taken from an amino acid sequence data base or a motif data base having the optimum correspondence to the input amino acid sequence; and

displaying by a display unit, the longest common subsequence (LCS) between the character sequence expressing the input amino acid sequence and the character sequence expressing the amino acid sequence having the optimum correspondence to the input amino acid sequence.

17. (Previously Presented) The method of claim 16, wherein determining the length of a longest common subsequence comprises:

selecting a character sequence expressing the input amino acid sequence of the target structure that has the optimum correspondence with a character sequence of the probe structure expressing an amino acid sequence taken from the amino acid sequence database or the motif database,

aligning the character sequence of the input amino acid sequence of the target structure with the character sequence of the probe structure having the optimum correspondence to determine the LCS and an occurrence position of the LCS, and

expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.

18-22. (Cancelled)

23. (Currently Amended) An apparatus for determining spatially similar portions of substances-a substance comprising amino acids by analyzing three-dimensional structures of a-the substance by dividing a molecule of the substance into a plurality of target subsets based on secondary structures and comparing each of the plurality of target subsets of the molecule of the substance to a plurality of probe subsets of by comparing a first probe structure, each of the plurality of probe subsets being expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets of secondary structures of probe structures, the-wherein a first subset of the plurality of probe subsets comprises comprising a first point set of an amino acid sequence database or a motif database and each of the plurality of target subsets is a target structure expressed by three-dimensional coordinates of elements belonging to a second subset of aof the plurality of target subsets of secondary structures of the-a target structure, wherein a first subset of the second plurality of target subsets subset comprisingcomprises a second point set of an input amino acid sequence of the target structure, wherein each point of the first point set and the second point set is expressed by three-dimensional coordinates and the coordinates are analyzed to determine correspondence, comprising:

a dividing unit to divide the second-target structure into a plurality of second-target subsets based on secondary structures of the three-dimensional coordinates of the target structure;

a determining unit to determine whether a correspondence is present between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure-by, for each subset of the plurality of target subsets of

secondary structures of the target structure:

generating a first tree structure for the first point set of the probe structure and a second tree structure for the second point set of the target structure wherein the tree structures are generated by successively giving correspondence to an element constituting the sets;

pruning the second tree structure for the second point set of the plurality of second subsets of the target structure in accordance with a predetermined pruning procedure; and

determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a-the same attribute, generating a correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure;

a calculating unit to

calculate a root mean square distance (RMSD) value between elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure to automatically determine a value for a distance between the elements of the first point set and the elements of the second point set, wherein substances expressed by a point set A={a₁, a₂, ..., a_i, ..., a_m} of a target subset, and a point set B={b₁, b₂, ..., b_j, ..., b_n} of a probe subset, wherein a_i (i=1, 2, ..., m) and b_j (j=1, 2, ..., n) are vectors expressing positions of respective elements in three-dimensional space, elements constituting substances A and B are related to each other, and the substance B is rotated and moved so that the r.m.s.d. value between corresponding elements is minimized in accordance with a following equation (1) wherein U denotes a rotation matrix and W_k denote respective weights:

$$R.M.S.D. = \frac{\left(\sum_{k=1}^n (w_k (U b_k - a_k)^2) \right)^{\frac{1}{2}}}{n}$$

.....(1);

determine whether the RMSD value is less than or equal to a predetermined threshold value set by a user, and where the RMSD value is less than or equal to a-the predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

determine a length of a longest common subsequence (LCS) between a

character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence taken from an amino acid sequence data base or a motif data base having the optimum correspondence to the input amino acid sequence; and

a display unit to

display the longest common subsequence (LCS) between the character sequence expressing the input amino acid sequence and the character sequence expressing the amino acid sequence having the optimum correspondence to the input amino acid sequence.

24. (Currently Amended) A computer-readable medium containing computer-readable instructions to determine spatially similar portions of substances a substance comprising amino acids by analyzing three-dimensional structures of a the substance by dividing a molecule of the substance into a plurality of target subsets based on secondary structures and comparing each of the plurality of target subsets of the molecule of the substance to a plurality of probe subsets of by comparing a first probe structure, each of the plurality of probe subsets being expressed by three-dimensional coordinates of elements belonging to a first subset of a plurality of subsets of secondary structures of probe structures, the wherein a first subset of the plurality of probe subsets comprising comprises a first point set of an amino acid sequence database or a motif database and each of the target subsets is a target structure expressed by three-dimensional coordinates of elements belonging to a second subset of aof the plurality of target subsets of secondary structures of the a target structure, wherein a first subset of the second plurality of target subset subsets comprising comprises a second point set of an input amino acid sequence of the target structure, the computer-readable instructions, wherein each point of the first point set and the second point set is expressed by three-dimensional coordinates and the coordinates are analyzed to determine correspondence, comprising:

dividing the target structure into a plurality of target subsets, wherein the first subset of the plurality of target subsets comprises a second point set expressing a position of an amino acid of the input amino acid sequence into a plurality of second subsets according to a secondary structure of the target structure exhibited by the three-dimensional coordinates of the elements of the second point set;

determining whether a correspondence is present between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure by, for each target subset of the plurality of target subsets of secondary structures of the target structure:

generating a first tree structure for the first point set of the probe structure and a

second tree structure for the second point set of the target structure wherein the tree structures are generated by successively giving correspondence to an element constituting the sets;

pruning the second tree structure for the second point set of the plurality of second subsets of the target structure in accordance with a predetermined pruning procedure; and

determining whether the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have a same attribute, and if the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure have athe same attribute, generating a correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure; and

calculating a root mean square distance (RMSD) value between elements corresponding in the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure to automatically determine a value for a distance between the elements of the first point set and the elements of the second point set, wherein substances expressed by a point set A={ $a_1, a_2, \dots, a_i, \dots, a_m$ } of a target subset, and a point set B={ $b_1, b_2, \dots, b_j, \dots, b_n$ } of a probe subset, wherein a_i ($i=1, 2, \dots, m$) and b_j ($i=1, 2, \dots, n$) are vectors expressing positions of respective elements in three-dimensional space, elements constituting substances A and B are related to each other, and the substance B is rotated and moved so that the r.m.s.d. value between corresponding elements is minimized in accordance with a following equation (1) wherein U denotes a rotation matrix and W_k denote respective weights:

$$r.m.s.d. = \frac{\left(\sum_{k=1}^n (w_k (Ub_k - a_k)^2) \right)^{\frac{1}{2}}}{n} \quad | \dots \dots (1);$$

determining whether the RMSD value is less than or equal to a predetermined threshold value set by a user, and where the RMSD value is less than or equal to athe predetermined threshold value, generating an optimum correspondence between the first point set of the probe structure and the second point set of the plurality of second subsets of the target structure;

determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence taken from an amino acid sequence data base or a motif data base having the optimum correspondence to the input amino acid sequence; and

displaying by a display unit, the longest common subsequence (LCS) between the character sequence expressing the input amino acid sequence and the character sequence expressing the amino acid sequence having the optimum correspondence to the input amino acid sequence.

25. (Previously Presented) The computer-readable medium of claim 24, wherein determining the length of a longest common subsequence comprises:

selecting a character sequence expressing the input amino acid sequence of the target structure that has the optimum correspondence with a character sequence of the probe structure expressing an amino acid sequence taken from the amino acid sequence database or the motif database,

aligning the character sequence of the input amino acid sequence of the target structure with the character sequence of the probe structure having the optimum correspondence to determine the LCS and an occurrence position of the LCS, and

expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.

26. (Withdrawn) A computer-readable medium containing computer-readable instructions to compare spatially similar portions of an input amino acid sequence and an amino acid sequence taken from an amino acid sequence database or a motif database, the computer-readable instructions comprising:

searching the amino acid sequence database and the motif database for an amino acid sequence or sequences having at least a predetermined degree of similarity to the input amino acid sequence;

determining a length of a longest common subsequence (LCS) between a character sequence expressing the input amino acid sequence and a character sequence expressing the amino acid sequence having a greatest degree of similarity to the input amino acid sequence, wherein the amino acid sequence having the greatest degree of similarity is selected from a set of amino acid sequences having at least the predetermined degree of similarity;

determining the LCS and an occurrence position of the LCS between the character sequence expressing the input amino acid sequence and the character sequence having the greatest degree of similarity and expressing an amino acid sequence taken from the amino acid sequence database or the motif database; and

aligning the character sequence of the input amino acid sequence with the character

sequence having the greatest degree of similarity and expressing the amino acid sequence from the amino acid sequence database or the motif database, based on the LCS and the occurrence position of the LCS, by inserting a blank corresponding to a length of a character sequence between positions of subsequences.